Initial Growth of the Rayleigh-Taylor Instability via Molecular Dynamics

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Molecular dynamics (MD) is a material simulation technique in which Newton's equations of motion for a large number of interacting particles are solved numerically [1]. In recent years, there has been increasing interest in the simulation of various problems in fluid dynamics using MD (and other atomistic methods) rather than the more traditional continuum techniques based on the Navier-Stokes equations [2-6]. The advantages of MD stem from the fundamental nature of the processes upon which it is based, as well as the fact that it includes the thermal fluctuations present in real fluids and that are lacking in most continuum solvers. The main disadvantage is the computational cost associated with the large number of particles present in most MD simulations. The microscale thermal fluctuations captured by MD allow us to directly probe the emergence of macroscopic hydrodynamic quantities as averages over the molecular randomness that underpins real-world fluids. In this highlight, we describe such an investigation in the context of the initial growth behavior of the Rayleigh-Taylor instability (RTI) [6].

The RTI occurs when a heavy fluid lies on top of a light fluid in the presence of a gravitational field g. This arrangement is unstable, and the two fluids subsequently combine in an archetypical example of turbulent fluid mixing. Figure 1 shows several stages in the early development of the RTI in an MD simulation with quasi-2D (or "thin slab") geometry. Given an initial interface between the two fluids possessing only small deviations from perfect flatness, it can be shown that the amplitude of a perturbation of wave number k will grow exponentially in time for small t as $A_k(t) = A_k(0)\exp[n(k)\,t]$. In his 1961 book *Hydrodynamic and Hydromagnetic Stability* [7], Chandrasekhar derived, via linearization of the incompressible Navier-Stokes equations, a function f such that the growth rate spectrum $n(k)$ satisfies $f(n(k), k) = 0$. This equation can be solved numerically to yield continuum-based predictions for the shape of $n(k)$. In particular, note that $n(k)$ has a maximum at k_{max}, known as the mode of maximum instability. In addition, for the systems with surface tension we consider here, $n(k)$ has a cutoff at k_{cut}, at which $n(k)$ passes from positive to negative.

The growth-rate spectrum of the RTI can be measured directly in MD simulations by taking Fourier transforms of the early development of the interface. We have performed such an analysis for a sequence of MD simulations, each describing a quasi-2D domain approximately 1 µm in width by 0.2 µm in height and containing approximately 2,000,000 Lennard-Jones particles. Due to the small length scales considered, it was necessary for the gravity g to be very large in order for the instability to develop in a reasonable number of time steps. The three values for g considered were $g = 2.7 \times 10^{10}\, g_{Earth}$, $g = 1.3 \times 10^{10}\, g_{Earth}$, and $g = 0.3 \times 10^{10}\, g_{Earth}$. The presence of entirely physical fluctuation-induced variations in the growth rate spectrum from one simulation to the next necessitated that we perform many runs at each gravity to obtain an adequate average $n(k)$ for comparison with Chandrasekhar's prediction. The results are shown in Fig. 2. Note that despite the vastly different levels of description between the MD simulations and the continuum theory, the agreement between the two is quite good. To within fluctuations, MD captures both the existence and value of the mode of maximum instability k_{max}, as well as the presence of the cutoff wave number k_{cut}. At large values of k, there is some discrepancy between the growth rate values manifested by MD and the theoretical predictions. This can

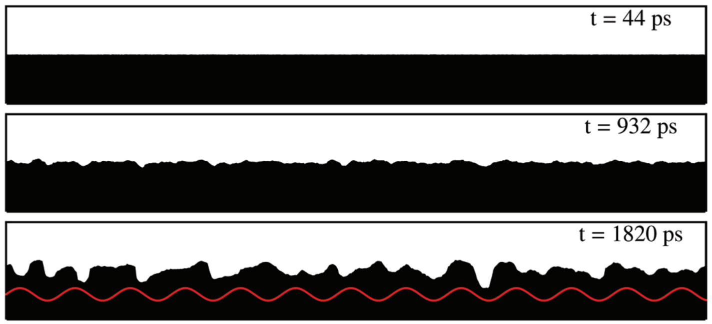

Fig. 1. Three snapshots from the initial stages of the Rayleigh-Taylor instability as simulated by MD. The red curve in the last frame is a reference sine curve of wavelength $\lambda_{max} = 2\pi/k_{max}$, illustrating that modes near the mode of maximum instability quickly dominate the shape of the interface.

be attributed to a number of factors, including the existence of nonexponential oscillations of the interface and the presence of nonlinear transport effects for low-wavelength disturbances.

In addition to the mean growth rate $n(k)$, it is instructive to consider the physical variation $\Delta n(k)$ in the growth rate as a function of k. This quantity is graphed in Fig. 3 for each of the three gravities we considered, along with a curve representing a polynomial fit to the low-k segment of all three sets of data to aid in recognizing the general trend. The important point to note is that the physical spread in the growth rate with respect to its mean is a monotonically increasing function of the wave number k (i.e., a decreasing function of the wavelength λ). Since the predicted mean is derived from purely hydrodynamic considerations, this is a clear demonstration that the validity of the Navier-Stokes equations emerges statistically as an average over the microscopic fluctuations in a fluid, and that individual instances of real fluid systems deviate from this average to an increasing degree as smaller scales are considered.

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[1] M. Allen, D. Tildesley, *Computer Simulation of Liquids,* Oxford Science Publications (1987).
[2] M. Mareschal, E. Kestemont, *Nature* **329,** 427-429 (1987).
[3] D.C. Rapaport, *Phys. Rev. E* **73,** 025301(R) (2006).
[4] K. Kadau et al., *Proc. Nat. Acad. Sci.* **101,** 5851-5855 (2004).
[5] K. Kadau et al., *Proc. Nat. Acad. Sci.* **104,** 7741-7745 (2007).
[6] J.L. Barber et al., *Eur. Phys. J. B* **64,** 271-276 (2008).
[7] S. Chandrasekhar, *Hydrodynamic and Hydromagnetic Stability,* Dover (1961).

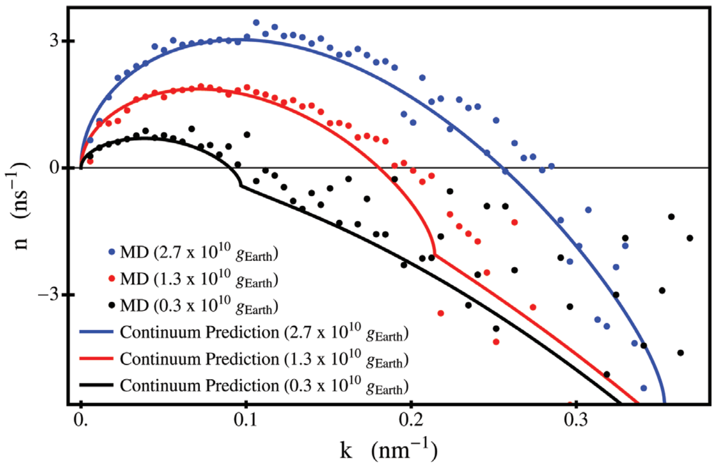

Fig. 2. Growth-rate spectra from MD simulations for each of the three gravities considered, along with the corresponding predictions from continuum theory.

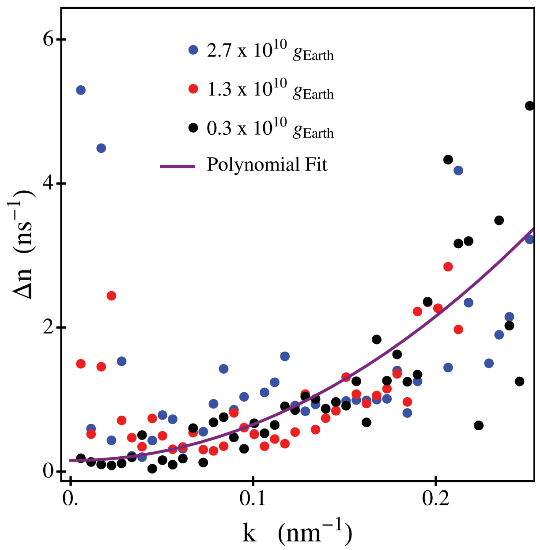

Fig. 3. Physical variation in the growth rate as a function of k from MD simulations, along with a curve representing a rough polynomial fit to the moderate-k segment of the data. Note that the apparent increase in $\Delta n(k)$ at very small k is an artifact of the periodic boundary conditions we employed and may be ignored.

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